Los Alamos National Laboratory LA-UR-19-22405

Los Alamos Updates to nuclear data evaluations

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Overview:

- ✓ Light element evaluations
- ✓ ²⁰⁸Pb evaluation
- ✓ Minor actinide evaluations
- ✓ Summary

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LANL Light-element (LE) evaluations

- Multichannel, unitary: fit all reaction/scattering data simultaneously
- Fit quantum mechanical amplitudes, not cross sections
- Superior to single-channel & cross-section curve fitting
- High-fidelity, low chi-squared: $\chi^2/DOF \sim 1.2 1.5$

Core capabilities/efforts

- LANL lead contributor LE evaluations for ENDF/B-VIII.0 (see table below)
- LE evaluations for many users/formats (ENDF, NJOY, ACE, NDI, etc.)
- Provide covariance information for all LE evaluations
- International efforts (IAEA Consultant's Meeting R-matrix evaluations/Standards)

Catalogue of some light-element evaluations

	H1	H2	H3	He3	He4	Li6	Li7
n	VIII.0	VII.1	VII.1	VII.1	VII.1	VIII.0	VII.1
р	VII.1	VII.1	VII.1	VII.1	2011*	VII.1	2001*
d		VII.1	VII.1, 2018	VII.1	2011	VII.1	2003*
t			VII.1	VII.1	2011*	VII.1	*
³ He				2001	2011*	VII.1	
α					2011*		

NCSP evaluations of interest

• NN, ⁹Be, ^{12/13}C, ¹⁶O

EDA Code Modernization

- NCSP FY20 request
- Higher-energies (<20 MeV)
- Interface EDA & NJOY, etc.

Roman numerals refer to ENDF versions

- -- All LANL evaluations except *
- -- * denote LLNL evaluations

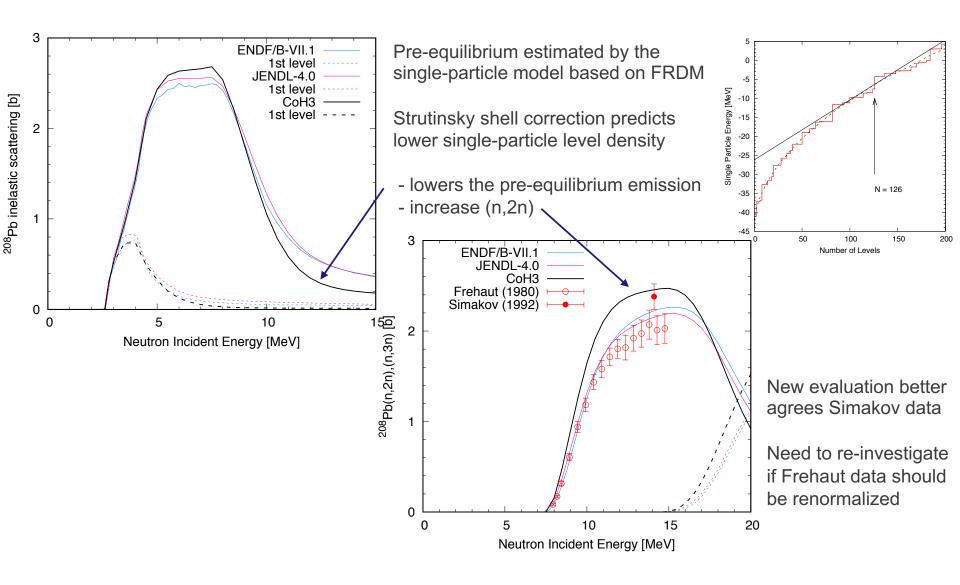
CoH₃: Coupled-Channes Hauser-Feshbach code

- Hauser-Feshbach-Moldauer therory for compound nucleus reaction
 - 45,000 lines C++ code (~ 140 C++ source files, ~60 headers, ~80 classes)
 - maintain by GNU Autotools package
- Modules and Models employed
- spherical and deformed optical models
- DWBA for direct inelastic scattering
- Moldauer's width fluctuation correction with LANL parametrization
- Gilbert-Cameron level density with updated parameters
- pre-equilibrium 2-component exciton model
- Madland-Nix prompt fission neutron spectrum including pre-fission emission
- direct/semidirect capture model
- mean-field models (FRDM and Hartree-Fock BCS)

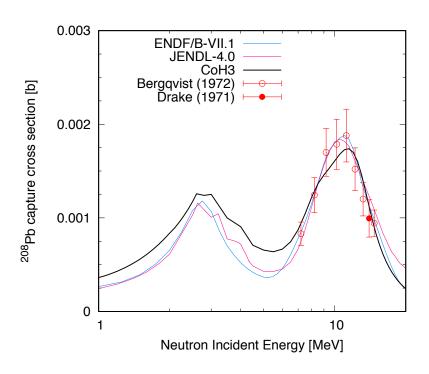
Consistent evaluations in all channels

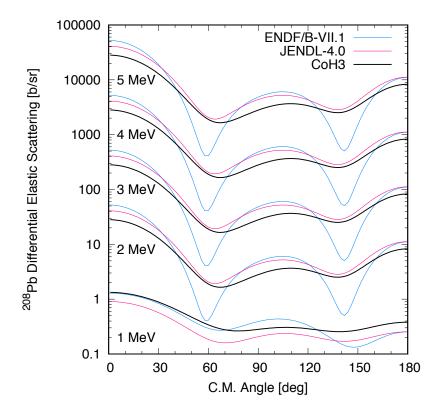


CoH₃ New Evaluation of ²⁰⁸Pb, (n,n'), (n,2n), and (n,3n)



CoH₃ New Evaluation of ²⁰⁸Pb, Capture and Elastic



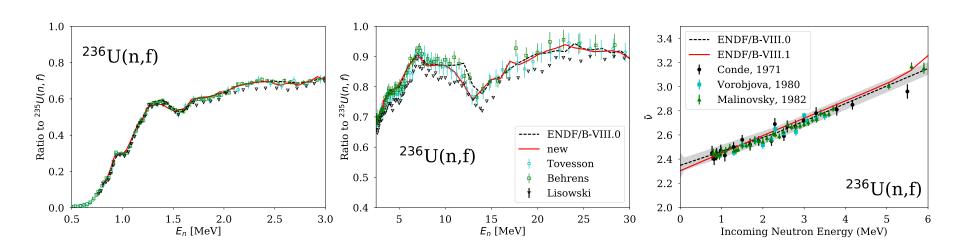


Very small capture cross section Realistic Direct/Semidirect capture theory applied (evaluations are simple Lorentzians)

Unphysical dips near 60 and 140 degrees removed Evaluation similar to JENDL-4

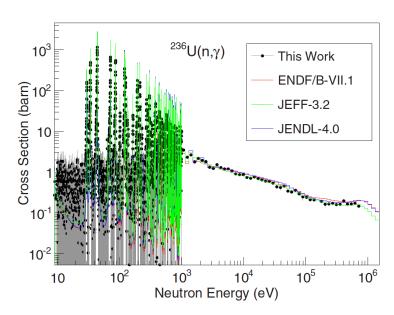
Evaluation of ^{234,236}U

- > Extensive and consistent evaluations based on CoH3 calculations, with parameters adjusted to experimental data (DANCE, WNR)
- All open channels included
- KALMAN-based evaluation for fission channel to include cross section data from WNR
- ≥ 234U: re-evaluation of nubar, consistent PFNS.
- > ²³⁶U: re-evaluation of nubar above 2nd chance fission, PFNS
- ➤ PFGS and gamma multiplicity taken from the recent ²³⁵U evaluation

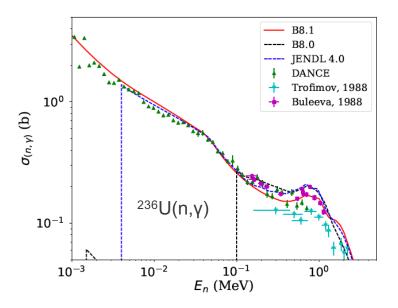


Evaluation ^{234,236}U (capture)

- Resonance parameters for ²³⁶U(n,γ) refitted to DANCE data, but only for the s wave and in different format than currently in ENDF (new fit this summer?)
- > Data for ²³⁴U(n,γ) will be analyzed this summer (before September?)
- ➤ CoH₃ evaluation
 - Width corrections fluctuation of Moldauer, with the Engelbrecht-Weidenmüller transformation (strict treatment of the directly coupled channels in the Hauser–Feshbach theory), the coupled-channels optical potential of Soukhovitskii
 - Same parameters used for the suite of U isotopes

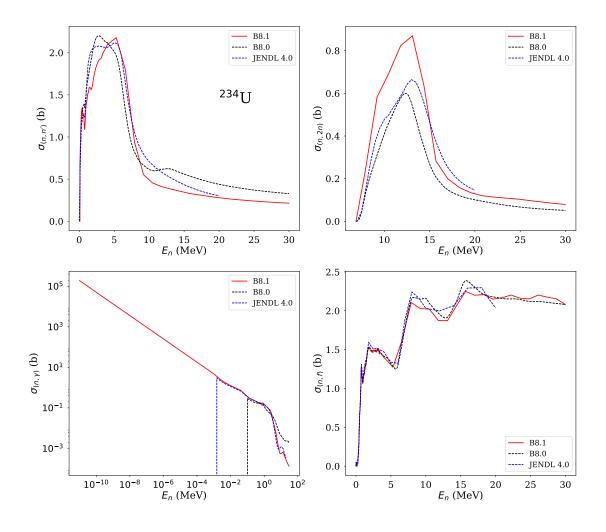


Baramsai et al, PRC 96 (2017) 024619



CoH₃ evaluation

²³⁴U evaluation: all channels consistent from CoH₃ calculations



New paradigm for nuclear data evaluations

•Novelty in evaluation procedure:

- Include >1000 integral experiments of various types
- Develop infrastructure for re-adjustment of existing evaluations each time any evaluation is changed

Prerequisites

- Reliable set of integral experiments (with input decks)
- Library of inputs and scripted procedures allowing for quick re-evaluation
- ML techniques for tracing outliers (in experiments and evaluations), for performing global adjustment and analysis of the results
- Reaction modeling adequate to reproduce experimental data (all reaction mechanisms)
- Extensive set of sensitivities
- Automated validation
- Integration of experimental, evaluation and validation communities

Benefits

- Accounting for differential and integral exp. on the same footing
- Extensive set of covariances including cross-material correlations
- Reduction of error compensation
- Improved responsiveness to new measurements and model advances

Summary

- Extend light-element evaluations: higher energy via code modernization
- ❖ Improved evaluation for ²⁰⁸Pb
- ❖ Complete and consistent evaluations for ^{234,236}U
- CoH3: extensive (many models) and flexible evaluation tool neutron induced reactions on medium and heavy nuclei
- ❖ New evaluation scheme using ML algorithms

Work in progress:

- Identify benchmarks that include ²³⁴U/²³⁶U and check the performance of the evaluation
- Include the s-wave parameters for $^{236}U(n,\gamma)$ (DANCE)
- Compare with $^{234}U(n,y)$ cross section, when the analysis is finished
- Neudecker: updates of PFNS for U and Pu based on new ChiNu data
- Kawano, Stetcu, Talou: new deterministic Hauser-Feschbach cascade model for PFNS/PFGS
- Adjustments to CGMF parameters so it can be used in future evaluations